Fourth Picture in Quantum Mechanics*

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(Received 19 February 1970)

A quantum-mechanical counterpart to the classical mechanical variation of constants method is derived, with initial values of coordinates and momenta as "constants." Use is made of a formal operator solution for nonautonomous or autonomous systems in classical mechanics, which we published earlier, and of the correspondence between Poisson brackets and commutators. An alternative unified Lie-algebraic derivation is also given. It is shown that the Schrödinger, Heisenberg, and interaction pictures in quantum mechanics do not correspond directly to the method of classical mechanical variation of these "constants." A fourth picture, termed "mixed interaction," is introduced and shown to so correspond. It complements the previous three in a symmetrical manner, bearing the same relation to the Heisenberg picture that the Schrödinger picture bears to the interaction one. The group-theoretic relationship to the interaction picture is noted, as is the relation to the usual variation-of-constants method in wave mechanics. For completeness, the classical counterparts of the Heisenberg and interaction pictures are also given. The present results arose from a comparison of quantum and classical treatments of collisions.

I. INTRODUCTION

In quantum mechanics the three pictures frequently employed are, as is well known, the Schrödinger, Heisenberg, and interaction (Dirac) pictures,[1] while in classical mechanics a commonly used method is that of variation of constants.[2] In a detailed comparison of a classical and quantum-mechanical perturbation treatment of transient phenomena (collisions), with initial values of coordinates and momenta as the "constants," we noticed that none of the three pictures corresponded directly to the cited classical method. In this paper we establish this point and, in the process, derive a fourth picture for quantum mechanics, i.e., one which provides the correspondence and which complements in a symmetrical manner the three customary pictures. It bears the same relation to the Heisenberg picture that the Schrödinger picture bears to the interaction picture. To avoid confusion with the usual variation of constants method[3] in quantum mechanics, which differs from the present one, we call the present method the "mixed-interaction picture" and denote it by M.

The essential features of the analysis are outlined in Sec. II. The classical mechanical variation of constants method and a formal solution are summarized in Sec. III, the quantum-mechanical counterpart is obtained by correspondence of Poisson brackets and commutators in Sec. IV, and a unified Lie-algebraic derivation of the classical and quantum expressions is given in Sec. V. The classical counterpart of the Heisenberg and interaction pictures is derived for completeness in Appendix A.

In Sec. V, a group-theoretic relationship [denoted there by (ii)] is noted between evolution operators for observables in the mixed-interaction picture and for wavefunction in the interaction picture. The relationship is similar to that between evolution operators for observables in the Heisenberg picture and for wavefunction in the Schrödinger picture.

The notation used in the present paper is discussed at some length in Appendix B.

II. DERIVATION IN BRIEF

In a classical mechanical variation of constants method, with initial values of coordinates and momenta as "constants," the original variables q_i and p_i (conjugate coordinates and momenta) are allowed to evolve via an unperturbed Hamiltonian $H_0(t)$, from initial values denoted by q_i^M and p_i^M, at time t_0. The evolution may be described in terms of a single equation involving an arbitrary C^∞ (i.e., infinitely differentiable) function f of q_i and p_i:

$$f(q,p)=(T^*(t)f)(q^M,p^M), \qquad (2.1)$$

where $T^*(t)$, the relevant time-evolution operator, is unity initially. q and p denote the totality of q_i's and p_i's $(i=1,\cdots,N)$; q^M and p^M denote the totality of q_i^M's and p_i^M's. The notation in (2.1) indicates that the function $T^*(t)f$ is evaluated at the point (q^M,p^M) in a $2N$-dimensional space. An explicit expression for $T^*(t)$ has been given in terms of multiple Poisson brackets involving H_0.[4] The asterisk and other symbols in (2.1) are discussed in Appendix B.

The q_i^M and p_i^M, which are constants of the motion in the unperturbed problem, evolve in time in the perturbed problem from initial values q_i^0 and p_i^0. They satisfy[4]

$$df(q^M,p^M)/dt=\{f(q^M,p^M),H_1(q,p,t)\}, \qquad (2.2)$$

where H_1 is the perturbation and $\{\ ,\ \}$ denotes a Poisson bracket. The q and p in H_1 are expressed in terms of q^M and p^M using (2.1), before integrating (2.2).

The quantum-mechanical counterpart to Eq. (2.2), obtained by Dirac's correspondence[5] of brackets and commutators, is

$$i\hbar df(\mathbf{q}^M,\mathbf{p}^M)/dt=[f(\mathbf{q}^M,\mathbf{p}^M),H_1(\mathbf{q},\mathbf{p},t)], \qquad (2.3)$$

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where $f(\mathbf{q}^M, \mathbf{p}^M)$ represents an arbitrary admissable operator-valued function of $(\mathbf{q}^M, \mathbf{p}^M)$. (Boldface type will be used for the q's and p's to avoid confusion of classical and quantum symbols.) Using the quantum-mechanical counterpart of (2.1), it can be shown that

$$[f(\mathbf{q}^M, \mathbf{p}^M), H_1(\mathbf{q}, \mathbf{p}, t)] = [f, U_0{}^\dagger H_1(t) U_0](\mathbf{q}^M, \mathbf{p}^M), \tag{2.4}$$

where U_0 is the usual evolution operator for the wavefunction of the unperturbed problem [Hamiltonian $H_0(t)$]. In Eq. (4), $[f, U_0{}^\dagger H_1(t) U_0]$ is evaluated at the point $(\mathbf{q}^M, \mathbf{p}^M)$. Since $U_0{}^\dagger H_1(t) U_0$ is usually denoted by $H_1{}^I(t)$,[6] the right-hand side of (2.4) can be written as $[f, H_1{}^I(t)](\mathbf{q}^M, \mathbf{p}^M)$, and latter introduced into (2.3).

Equation (2.3) can be integrated, and the solution is found to be (as may also be verified by direct substitution)

$$f(\mathbf{q}^M, \mathbf{p}^M) = (U_I{}^\dagger f U_I)(\mathbf{q}^0, \mathbf{p}^0), \tag{2.5}$$

where U_I denotes $U_I(t, t_0)$ and is the evolution operator in the usual interaction picture,[7] $U_I(t_0, t_0)$ is unity, and $U_I{}^\dagger f U_I$ is evaluated at the point $(\mathbf{q}^0, \mathbf{p}^0)$.

The quantum-mechanical picture corresponding to the variables $\mathbf{q}_i{}^M$ and $\mathbf{p}_i{}^M$ is readily deduced. Since expectation values are invariant to a unitary transformation, we have

$$\langle \psi_S | f(\mathbf{q}^0, \mathbf{p}^0) | \psi_S \rangle = \langle \psi_M | f(\mathbf{q}^M, \mathbf{p}^M) | \psi_M \rangle, \tag{2.6}$$

where ψ_S and ψ_M are the wavefunctions in the Schrödinger and mixed-interaction pictures. Introduction of (2.5) shows that

$$\langle \psi_S | f(\mathbf{q}^0, \mathbf{p}^0) | \psi_S \rangle = \langle \psi_M | (U_I{}^\dagger f U_I)(\mathbf{q}^0, \mathbf{p}^0) | \psi_M \rangle, \tag{2.6$'$}$$

and, thus, that

$$\psi_S(q, t) = U_I(t, t_0)\psi_M(q, t). \tag{2.7}$$

Inasmuch as $\psi_I(q, t)$ equals $U_I(t, t_0)\psi_H(q)$, where $\psi_I(q, t)$ and $\psi_H(q)$ are the wavefunctions in the interaction and Heisenberg pictures, the mixed-interaction picture bears the same relation to the Schrödinger picture that the Heisenberg picture does to the interaction one. The evolution operator $U_M(t, t_0)$ is defined by

$$\psi_M(q, t) = U_M(t, t_0)\psi_M(q, t_0). \tag{2.8}$$

Since $\psi_S(q, t)$ equals $U(t, t_0)\psi_S(q, t_0)$, and since $\psi_S(q, t_0)$, $\psi_M(q, t_0)$, and $\psi_H(q)$ are all equal, (2.7) and (2.8) yield

$$U_M(t, t_0) = U_I{}^\dagger(t, t_0) U(t, t_0) = U^\dagger(t, t_0) U_0(t, t_0) U(t, t_0). \tag{2.9}$$

Thereby, the mixed-interaction picture differs from the other three.

In terms of an expansion in eigenfunctions of φ_n of a time-independent Hamiltonian H_0, we have

$$\begin{aligned} \psi_H &= \sum a_n(t_0)\varphi_n, \\ \psi_M &= \sum a_n(t_0)\varphi_n \exp[-i(t-t_0)E_n/\hbar], \\ \psi_I &= \sum a_n(t)\varphi_n, \\ \psi_S &= \sum a_n(t)\varphi_n \exp[-i(t-t_0)E_n/\hbar]. \end{aligned} \tag{2.10}$$

Thus, the fourth picture complements in a symmetrical way the three customary pictures.

The customary variation-of-constants method in quantum mechanics involves obtaining equations for variation of the $a_n(t)$'s and so [as is seen from (2.10)] corresponds to a calculation in the interaction picture.[8]

III. CLASSICAL MECHANICAL VARIATION OF CONSTANTS

We recall now the method of variation of constants in classical mechanics[2] and a formal solution[4] in more detail. The canonically conjugate coordinates and momenta, q_i and p_i, are first expressed in terms of some constants of the motion, $q_i{}^M$ and $p_i{}^M$, of the unperturbed problem. In this paper we choose $q_i{}^M$ and $p_i{}^M$ to be the initial values of q_i and p_i. Thereby, one first solves the equations of motion for the dynamical path $(q_i(t), p_i(t))$ in the following unperturbed problem:

$$\begin{aligned} dq_i/dt &= \partial H_0(q, p, t)/\partial p_i, \\ dp_i/dt &= -\partial H_0(q, p, t)/\partial q_i, \\ q_i = q_i{}^M, &\quad p_i = p_i{}^M \quad (t = t_0), \end{aligned} \tag{3.1}$$

where $H_0(q, p, t)$ is the Hamiltonian of the unperturbed problem. In terms of Poisson brackets, (3.1) can be rewritten as

$$\begin{aligned} dq_i/dt &= \{q_i, H_0(q, p, t)\}, \\ dp_i/dt &= \{p_i, H_0(q, p, t)\}, \\ q_i = q_i{}^M, &\quad p_i = p_i{}^M \quad (t = t_0). \end{aligned} \tag{3.2}$$

Any C^∞ function of q and p, $f(q, p)$, varies with time because q and p are time dependent:

$$\frac{df(q, p)}{dt} = \sum_i \left[\left(\frac{\partial f(q, p)}{\partial q_i}\right)\left(\frac{dq_i}{dt}\right) + \left(\frac{\partial f(q, p)}{\partial p_i}\right)\left(\frac{dp_i}{dt}\right)\right]. \tag{3.3}$$

Equations (3.1) and (3.3) yield

$$\begin{aligned} df(q, p)/dt &= \{f(q, p), H_0(q, p, t)\}, \\ q_i = q_i{}^M, &\quad p_i = p_i{}^M \quad (t = t_0). \end{aligned} \tag{3.4}$$

The advantage of using (3.4) compared with (3.1) is that it leads to a coordinate-free description of the evolution, as in Eq. (3.9) below. As noted in Appendix B, (3.2) is a particular case of (3.4).

A perturbation $H_1(q, p, t)$ causes the "constants" of the motion of the unperturbed problem, $q_i{}^M$ and $p_i{}^M$, to vary with time.[2,4] Just as (3.1) led to (3.4), the

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equations of motions for $q_i^M(t)$ and $p_i^M(t)$ lead to

$$df(q^M, p^M)/dt = \{f(q^M, p^M), H_1(q, p, t)\}, \quad (3.5)$$
$$q_i^M = q_i^0, \quad p_i^M = p_i^0 \quad (t = t_0),$$

where the q and p in $H_1(q, p, t)$ denote the solution of (3.4); q_i^0 and p_i^0 denote the true initial values of q_i and p_i (i.e., the values at $t = t_0$) and hence of the q_i^M and p_i^M defined earlier.

The equations to be solved are (3.4) and then (3.5); in (3.5) the q_i's and p_i's are first expressed in terms of q_i^M's and p_i^M's using the solution to (3.4). Elsewhere, we have given a formal solution to (3.4) and (3.5) in operator form,[4] and we employ it there. To describe the solution, we define a function[9] B:

$$-B(C, t, t_0) = \int_{t_0}^{t} C_{t_1} dt_1 + \frac{1}{2} \int_{t_0}^{t} \left\{ C_{t_2}, \int_{t_0}^{t_2} C_{t_1} dt_1 \right\} dt_2$$
$$+ \frac{1}{4} \int_{t_0}^{t} \left\{ C_{t_3}, \int_{t_0}^{t_3} \left\{ C_{t_2}, \int_{t_0}^{t_2} C_{t_1} dt_1 \right\} dt_2 \right\} dt_3$$
$$+ \frac{1}{12} \int_{t_0}^{t} \left\{ \left\{ C_{t_3}, \int_{t_0}^{t_3} C_{t_2} dt_2 \right\}, \int_{t_0}^{t_3} C_{t_1} dt_1 \right\} dt_3 + \cdots, \quad (3.6)$$

where C_{t_i} is a function C at time t_i. It is also convenient to introduce a notation ad B of Lie-algebraic origin[10]:

$$\exp(\text{ad } B) \equiv 1 + \text{ad } B + (1/2!)(\text{ad } B)^2 + (1/3!)(\text{ad } B)^3 + \cdots$$
$$= 1 + \{B, \} + (1/2!)\{B, \{B, \}\} + (1/3!)\{B, \{B, \{B, \}\}\} + \cdots, \quad (3.7)$$

the ad B in (7) denoting the operator $\{B, \}$.

The formal solution[4] to (3.4) is (3.8), which also serves to identify the $T^*(t)$ in (2.1):

$$f(q, p) = \{[\exp \text{ad } B(H_0(t), t, t_0)] f\}(q^M, p^M), \quad (3.8)$$

where this B is the B in (3.6), with C_{t_i} replaced by $H_0(t_i)$. The q^M and p^M are treated as constants in (3.8).

When (3.8) is applied to $H_1(q, p, t)$, we have

$$H_1(q, p, t) = H_1^I(t)(q^M, p^M) \equiv H_1^I(q^M, p^M, t), \quad (3.9)$$

where $H_1^I(t)$ is defined as

$$H_1^I(t) = [\exp \text{ad } B(H_0(t), t, t_0)] H_1(t). \quad (3.10)$$

Equations (3.5) and (3.8) yield

$$df(q^M, p^M)/dt = \{f, H_1^I(t)\}(q^M, p^M), \quad (3.11)$$
$$q_i^M = q_i^0, \quad p_i^M = p_i^0, \quad t = t_0.$$

The formal solution to (3.11), and therefore to (3.5), can be written as[4]

$$f(q^M, p^M) = \{[\exp \text{ad } B(H_1^I(t), t, t_0)] f\}(q^0, p^0). \quad (3.12)$$

A classical mechanical variation of constants solution to the equations of motion of the perturbed problem is given by (3.8) and (3.12). This description is coordinate free: For example, according to (3.8), the dynamics can be described in terms of the evolution of a function f to a function $\{[\exp \text{ad } B(H_0(t), t, t_0)] f\}$, both evaluated at the initial point (q^M, p^M). Any point, (q^M, p^M) for example, is invariant to coordinate transformations.

IV. QUANTUM-MECHANICAL COUNTERPART TO CLASSICAL VARIATION OF CONSTANTS

To obtain the quantum-mechanical counterparts to Eqs. (3.4)–(3.12), we use Dirac's correspondence of Poisson brackets and commutators[5]

$$i\hbar\{ , \} \leftrightarrow [,]. \quad (4.1)$$

Later, a direct Lie-algebraic derivation of (4.14) and (4.15) is given instead. With use of (4.1), the quantum-mechanical counterparts to the previous equations can be written as

$$i\hbar df(\mathbf{q}, \mathbf{p})/dt = [f(\mathbf{q}, \mathbf{p}), H_0(\mathbf{q}, \mathbf{p}, t)], \quad (4.2)$$
$$\mathbf{q}_i = \mathbf{q}_i^M, \quad \mathbf{p}_i = \mathbf{p}_i^M \quad (t = t_0),$$
$$i\hbar df(\mathbf{p}^M, \mathbf{q}^M)/dt = [f(\mathbf{q}^M, \mathbf{p}^M), H_1(\mathbf{q}, \mathbf{p}, t)], \quad (4.3)$$
$$\mathbf{q}_i^M = \mathbf{q}_i^0, \quad \mathbf{p}_i^M = \mathbf{p}_i^0 \quad (t = t_0),$$

where the $\mathbf{q}$ and $\mathbf{p}$ in $H_1(\mathbf{q}, \mathbf{p}, t)$ denote the solution of (4.2), expressed in terms of $(\mathbf{q}^M, \mathbf{p}^M, t)$. A quantum-mechanical operator $\mathbf{B}$ is defined via (4.4). (This symbol will be the only boldfaced one, apart from the $\mathbf{q}$'s and $\mathbf{p}$'s, since here there could be some chance of confusion.)

$$-\mathbf{B}(C, t, t_0) = \frac{1}{i\hbar} \int_{t_0}^{t} C_{t_1} dt_1 + \frac{1}{2(i\hbar)^2}$$
$$\times \int_{t_0}^{t} \left[C_{t_2}, \int_{t_0}^{t_2} C_{t_1} dt_1 \right] dt_2 + \frac{1}{4(i\hbar)^3}$$
$$\times \int_{t_0}^{t} \left[C_{t_2}, \int_{t_0}^{t_3} \left[C_{t_2}, \int_{t_0}^{t_2} C_{t_1} dt_1 \right] dt_2 \right] dt_3 + \frac{1}{12(i\hbar)^3}$$
$$\times \int_{t_0}^{t} \left[\left[C_{t_3}, \int_{t_0}^{t_3} C_{t_2} dt_2 \right], \int_{t_0}^{t_3} C_{t_1} dt_1 \right] dt_3 + \cdots, \quad (4.4)$$

where C_{t_i} denotes $C(t_i)$. The following notation is also employed:

$$\exp \text{ad } \mathbf{B} \equiv 1 + \text{ad } \mathbf{B} + (1/2!)(\text{ad } \mathbf{B})^2 + (1/3!)(\text{ad } \mathbf{B})^3 + \cdots$$
$$= 1 + [\mathbf{B},] + (1/2!)[\mathbf{B}, [\mathbf{B},]] + (1/3!)[\mathbf{B}, [\mathbf{B}, \mathbf{B},]]] + \cdots. \quad (4.5)$$

Thereby, the adjoint operator denotes a commutator in quantum mechanics and a Poisson bracket in classical mechanics.

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The quantum-mechanical counterparts to (3.8), (3.12), and (3.10) then are

$$f(\mathbf{q},\mathbf{p})=\{[\exp \mathrm{ad}\,\mathbf{B}(H_0(t),t,t_0)]f\}(\mathbf{q}^M,\mathbf{p}^M) \quad (4.6)$$

and

$$f(\mathbf{q}^M,\mathbf{p}^M)=\{[\exp \mathrm{ad}\,\mathbf{B}(H_1{}^I(t),t,t_0)]f\}(\mathbf{q}^0,\mathbf{p}^0), \quad (4.7)$$

where

$$H_1{}^I(t)=\{[\exp \mathrm{ad}\,\mathbf{B}(H_0(t),t,t_0)]\}H_1(t) \quad (4.8)$$

and the notation has the same meaning that it did in classical mechanics. For example, in (4.6) the operator f, evaluated at a point $(\mathbf{q}(t),\mathbf{p}(t))$, equals $[\exp \mathrm{ad}\,\mathbf{B}(H_0(t),t,t_0)]f$, evaluated at the point $(\mathbf{q}^M,\mathbf{p}^M)$.

Equations (4.6)–(4.8) can be rewritten in terms of the familiar evolution operators $U_0(t,t_0)$ and $U_I(t,t_0)$, i.e., in terms of the solutions to

$$i\hbar dU_0(t,t_0)/dt=H_0(t)U_0(t,t_0), \quad (4.9)$$

$$i\hbar dU_I(t,t_0)/dt=(U_0{}^\dagger H_1(t)U_0)U_I(t,t_0), \quad (4.10)$$

by first noting that the solution to (4.9) is[11]

$$U_0(t,t_0)=\exp[-\mathbf{B}(H_0(t),t,t_0)]. \quad (4.11)$$

Application of a Baker–Hausdorff identity[12] to (4.8) and use of (4.11) then yield a well-known result,

$$H_1{}^I(t)=U_0{}^\dagger H_1(t)U_0. \quad (4.12)$$

The solution[11] to (4.10) is then

$$U_I(t,t_0)=\exp[-\mathbf{B}(H_1{}^I(t),t,t_0)]. \quad (4.13)$$

Equations (4.6) and (4.7) can now be rewritten, with the aid of the Baker–Hausdorff identity[12] as

$$f(\mathbf{q},\mathbf{p})=(U_0{}^\dagger fU_0)(\mathbf{q}^M,\mathbf{p}^M) \quad (4.14)$$

and

$$f(\mathbf{q}^M,\mathbf{p}^M)=(U_I{}^\dagger fU_I)(\mathbf{q}^0,\mathbf{p}^0), \quad (4.15)$$

which is the same as that cited earlier (2.5).

The arguments leading from (2.5) to (2.9) now apply and lead to the conclusions drawn in Sec. II regarding the mixed-interaction picture M. The fact that the series in (4.4) is a formal series, in that convergence questions have not been considered, does not affect the discussion in Sec. II.

The expressions for the operators in (4.6)–(4.13) simplify only when the relevant Hamiltonians are time independent. Normally, the only ones for which this situation can occur are H_0 and H. All commutators in (4.4) then vanish, and Eqs. (4.6), (4.11), and (2.9) become

$$\begin{aligned}f(\mathbf{q},\mathbf{p})&=[(\exp \mathrm{ad}\,i(t-t_0)H_0/\hbar)f](\mathbf{q}^M,\mathbf{p}^M)\\&=\{[\exp i(t-t_0)H_0/\hbar]f[\exp -i(t-t_0)H_0/\hbar]\}\\&\qquad\times(\mathbf{q}^M,\mathbf{p}^M), \quad (4.16)\end{aligned}$$

$$U_0(t,t_0)=\exp(-i(t-t_0)H_0/\hbar). \quad (4.17)$$

$$\begin{aligned}U_M(t,t_0)&=[\exp i(t-t_0)H/\hbar][\exp -i(t-t_0)H_0/\hbar]\\&\qquad\times[\exp -i(t-t_0)H/\hbar]. \quad (4.18)\end{aligned}$$

V. LIE-ALGEBRAIC DERIVATION

The results in the Sec. IV were derived from the classical ones in Sec. III using the correspondence between Poisson brackets and commutators. Equations (3.8), (3.12), (4.6), and (4.7), classical and quantum, are derived in the present section in a unified algebraic manner instead.

The canonically conjugate variables in any of the preceding equations are denoted by $x_1,\cdots,x_{2N}$ [e.g., the q_i's and p_i's in (3.4)], and form a $2N$-dimensional vector space. The equations of motion in Sec. III or Sec. IV can be written as

$$df(x)/dt=-\mathrm{ad}\,\mathcal{H}(x,t)f(x), \quad (5.1)$$

where ad denotes a Lie bracket, which is the Poisson bracket in the classical case and the commutator in the quantum one. $\mathcal{H}(x,t)$ is the appropriate Hamiltonian. For example, in Eq. (3.4) $\mathcal{H}(x,t)$ is $H_0(q,p,t)$. When (3.4) is solved, as in the manner given below, the $H_1(q,p,t)$ in (3.5) then becomes $H_1{}^I(q^M,p^M,t)$, which in turn becomes the $\mathcal{H}(x,t)$ for (3.11). Similarly, in Eq. (4.2) $\mathcal{H}(x,t)$ would be $H_0(\mathbf{q},\mathbf{p},t)/i\hbar$ while the solution of (4.2) (as given below) would then convert the $H_1(\mathbf{q},\mathbf{p},t)/i\hbar$ in (4.3) to $H_1{}^I(\mathbf{q}^M,\mathbf{p}^M,t)/i\hbar$, which in turn becomes $\mathcal{H}(x,t)$ for that equation.

An operator ad $\mathcal{H}(t)$ can be defined for later use by rewriting Eq. (5.1) as

$$df(x)/dt=-[\mathrm{ad}\,\mathcal{H}(t)f](x). \quad (5.2)$$

A solution of (5.1) is given below. It is a Lie-algebraic extension of the method which we used in Ref. 4 for classical mechanics (and for other systems of ordinary differential equations). In Ref. 4 the present Eqs. (5.3)–(5.4) were postulated and then justified *a posteriori*, but here they are derived instead.

If $\mathcal{H}(t)$ in (5.1) did not depend explicitly on time, integration would be immediate, the solution being

$$f(x)=([\exp[-(t-t_0)\mathrm{ad}\,\mathcal{H}]f])(x^0),$$

$$\mathcal{H} \text{ independent of } t, \quad (5.3)$$

where x^0 is the initial value of x, e.g., it is (q^M,p^M) in (3.4), (q^0,p^0) in (3.5), etc.

When $\mathcal{H}$ represents $H_1{}^I$, it normally depends explicitly on t, even when H_0 and H_1 do not. For an $\mathcal{H}(x,t)$ which is explicitly t dependent, the integration of (5.1) over a sufficiently very small interval $(t_0,t_0+\delta t)$ would again yield (5.3), but with $(t-t_0)$ replaced by δt. The value of $f(x)$ at $t_0+\delta t$ then serves as an initial value for a subsequent integration of (5.2) over an interval $t_0+\delta t$ to $t_0+2\delta t$, the integration of which yields another exponential.[13] In this way, $f(x)$ is ultimately expressed as a product of exponentials, members in fact of a Lie group. Such a product of Lie-group elements can be expressed as a single exponential of a sum of members of the corresponding Lie algebra (Baker–Campbell–Hausdorff theorem),[14] an algebra

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generated by the time-dependent infinitesimal generator ad $\mathcal{H}(t)$ as t varies. We may then write, instead of (5.3),

$$f(x)=(T^*(t)f)(x^0), \tag{5.4}$$

where

$$T^*(t)\equiv \exp \operatorname{ad} \mathcal{B}(t). \tag{5.5}$$

ad $\mathcal{B}(t)$ is a sum of Lie elements generated by ad $\mathcal{H}(t)$ as t varies, and is to be determined.

Some information is already available about ad $\mathcal{H}(t)$ and ad $\mathcal{B}(t)$: These elements are "derivations," regardless of whether the adjoint indicates a Poisson bracket or a commutator. We recall that when applied to a product, denoted by $f\circ g$, a derivation D is an operator satisfying[15]

$$D(f\circ g)=f\circ(Dg)+(Df)\circ g. \tag{5.6}$$

In the present instance we are interested in products which are Lie products, in which case (5.4) can be rewritten as

$$D((\operatorname{ad} f)g)=(\operatorname{ad} f)(Dg)+(\operatorname{ad}(Df))g. \tag{5.7}$$

On replacing D by ad $\mathcal{H}(t)$ or by ad $\mathcal{B}(t)$, Eq. (5.7) is seen to be merely Jacobi's identity[16], and so (5.7) and hence (5.6) are applicable in the present case.

Since the exponential of a derivation is known to convert products into products,[17] i.e., to be an automorphism, Eq. (5.5) now yields

$$T^*(t)(f\circ g)=(T^*(t)f)\circ(T^*(t)g). \tag{5.8}$$

Equation (5.8) is immediately extended to "polynomials" of $f(x)$, generated by the multiplication $\circ$: If $P_n(f(x))$ denotes such a polynomial, then it follows from repeated application of (5.8) that

$$P_n(f(x))=[P_n(T^*(t)f)](x^0)=(T^*(t)P_n(f))(x^0). \tag{5.9}$$

This result can then be extended to continuous functions of $f(x)$ using a well-known argument (polynomials are dense in the space of such functions). One such function is ad $\mathcal{H}(x,t)f(x)$. Hence,

$$\begin{aligned}\operatorname{ad}\mathcal{H}(x,t)f(x)&=(\operatorname{ad}\mathcal{H}(t)\,T^*(t)f)(x^0)\\&=(T^*(t)\operatorname{ad}\mathcal{H}(t)f)(x^0).\end{aligned} \tag{5.10}$$

Equations (5.1), (5.4), and (5.10) thus yield

$$[(dT^*(t)/dt)f](x^0)=-(T^*(t)\operatorname{ad}\mathcal{H}(t)f)(x^0). \tag{5.11}$$

Omission of the arbitrary initial point x^0 and then omission of the arbitrary function f yields

$$dT^*(t)/dt=-T^*(t)\operatorname{ad}\mathcal{H}(t). \tag{5.12}$$

This equation, with $T^*(t)$ replaced by a Y^{-1} and with ad $\mathcal{H}(t)$ replaced by a $-A(t)$, is now the same as that solved by Magnus[18] in Ref. 9, and his solution, applied to (5.12), yields a $T^*(t)$ given by (5.5) with ad $\mathcal{B}$ given by

$$\begin{aligned}-\operatorname{ad}\mathcal{B}=&\int_{t_0}^{t}\operatorname{ad}\mathcal{H}_{t_1}dt_1+\frac{1}{2}\int_{t_0}^{t}\Big[\operatorname{ad}\mathcal{H}_{t_2},\\&\times\int_{t_0}^{t_2}\operatorname{ad}\mathcal{H}_{t_1}dt_1\Big]dt_2+\frac{1}{4}\int_{t_0}^{t}\Big[\operatorname{ad}\mathcal{H}_{t_3},\\&\times\int_{t_0}^{t_3}\Big[\operatorname{ad}\mathcal{H}_{t_2},\int_{t_0}^{t_2}\operatorname{ad}\mathcal{H}_{t_1}dt_1\Big]dt_2\Big]dt_3\\&+\frac{1}{12}\int_{t_0}^{t}\Big[\Big[\operatorname{ad}\mathcal{H}_{t_3},\int_{t_0}^{t_3}\operatorname{ad}\mathcal{H}_{t_2}dt_2\Big],\\&\times\int_{t_0}^{t_3}\operatorname{ad}\mathcal{H}_{t_1}dt_1\Big]dt_3+\cdots,\end{aligned} \tag{5.13}$$

where ad $\mathcal{H}_{t_i}$ denotes ad $\mathcal{H}(t_i)$.

The solution to (5.1) is provided by (5.4), (5.5), and (5.13). The various equations derived in Sec. III and Sec. IV then also follow from this solution.

Several algebraic relationships in the M picture between the classical and quantum-evolution operators, whose application to collisional treatments is discussed separately, may be noted:

(i) The Lie algebra associated with the evolution of the classical q_i^M and p_i^M is identical with that for the evolution of the quantum $\mathbf{q}_i^M$ and $\mathbf{p}_i^M$, since both obey (5.1)–(5.13), with the correspondence (4.1). Further, this Lie algebra is the adjoint representation of that generated by $H_1^I(t)$ in the time evolution of $U_I^\dagger(t,t_0)$.[19]

(ii) The Hermitian adjoint $U_I^\dagger(t,t_0)$ of the evolution operator $U_I(t,t_0)$ for the wavefunction in the interaction picture is related to the evolution operator for arbitrary functions $f(\mathbf{q}^M,\mathbf{p}^M)$ of the "constants" in the M picture. Equations (4.13) and (4.15) show that the relationship is one of adjointness, in that

$$\begin{aligned}f(\mathbf{q}^M,\mathbf{p}^M)&=(U_I^\dagger(t,t_0)fU(t,t_0))(\mathbf{q}^0,\mathbf{p}^0)\\&=[(\operatorname{ad}U_I^\dagger(t,t_0))f](\mathbf{q}^0,\mathbf{p}^0),\end{aligned} \tag{5.14}$$

where the notation ad g for the adjoint of a group element g is described in Ref. 20.

The relationship in (ii) is similar to that between the Hermitian adjoint $U^\dagger(t,t_0)$ of the evolution operator $U(t,t_0)$ of the Schrödinger wavefunction $\psi_S(q,t_0)$ and the evolution operator, ad $U^\dagger(t,t_0)$, of the dynamical variables $(\mathbf{q},\mathbf{p})$ in the Heisenberg picture,

$$f(\mathbf{q},\mathbf{p})=(\operatorname{ad}U^\dagger(t,t_0)f)(\mathbf{q}^0,\mathbf{p}^0), \tag{5.15}$$

for the latter is an abbreviation for $(U^\dagger fU)(\mathbf{q}^0,\mathbf{p}^0)$.

Another relationship, reflecting (ii), between the mixed-interaction and interaction pictures is the following: In the mixed-interaction picture, variation of constants involves variation of observables $\mathbf{q}^M$ and $\mathbf{p}^M$. (There is no "variation of constants" $\mathbf{q}^I$ and $\mathbf{p}^I$ in the interaction picture, a fact clear in Appendix A, for

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example.) In the interaction picture, variation of constants involves variation of the wavefunction, e.g., variation of the $a_n(t)$'s in (2.10). [There is no "variation of constants" $a_n(t_0)$ in Eq. (2.10) in the mixed-interaction picture.]

ACKNOWLEDGMENT

It is a pleasure to acknowledge a helpful discussion with Professor K. T. Chen of the University of Illinois.

APPENDIX A: CLASSICAL COUNTERPARTS OF THE HEISENBERG AND INTERACTION PICTURES

A. Heisenberg Picture

The equations of motion are represented by

$$i\hbar \dot{f}(\mathbf{q}, \mathbf{p})/dt = [f(\mathbf{q}, \mathbf{p}), H(\mathbf{q}, \mathbf{p}, t)], \qquad \text{(A1)}$$

$$\mathbf{q}_i = \mathbf{q}_i^0, \quad \mathbf{p}_i = \mathbf{p}_i^0, \quad t = t_0,$$

whence application of the solution in Sec. V with ad $\mathcal{H}(x, t)$ being $[H(\mathbf{q}, \mathbf{p}, t), \;]$ yields

$$f(\mathbf{q}, \mathbf{p}) = \{[\exp \operatorname{ad} \mathbf{B}(H(t), t, t_0)]f\}(\mathbf{q}^0, \mathbf{p}^0) \qquad \text{(A2)}$$

whose classical counterpart, obtained by (4.1), is

$$f(q, p) = \{[\exp \operatorname{ad} B(H(t), t, t_0)]f\}(q^0, p^0). \qquad \text{(A3)}$$

B. Interaction Picture

Here, operators $\mathbf{q}_i^I$ and $\mathbf{p}_i^I$ are introduced, which evolve with time from initial values $\mathbf{q}_i^0$ and $\mathbf{p}_i^0$ via the unperturbed Hamiltonian, H_0, and in (A4) and (A5) several results are recalled:

$$i\hbar df(\mathbf{q}^I, \mathbf{p}^I)/dt = [f(\mathbf{q}_i^I, \mathbf{p}_i^I, t), H_0(\mathbf{q}^I, \mathbf{p}^I, t)], \qquad \text{(A4)}$$

$$\mathbf{q}_i^I = \mathbf{q}_i^0, \quad \mathbf{p}_i^I = \mathbf{p}_i^0, \quad t = t_0.$$

Also, in the interaction picture, when $\mathbf{q}^I$ and $\mathbf{p}^I$ evolve to $\mathbf{q}$ and $\mathbf{p}$, any admissible function f evolves according to

$$f(\mathbf{q}, \mathbf{p}) = (U_I^\dagger(t, t_0) f U_I(t, t_0))(\mathbf{q}^I, \mathbf{p}^I). \qquad \text{(A5)}$$

Unlike the $\mathbf{q}^M$ and $\mathbf{p}^M$, the $\mathbf{q}^I$ and $\mathbf{p}^I$ are not constants in the unperturbed problem.

The solution to (A4), obtained by the method of Sec. V, is

$$(\mathbf{q},^I f \mathbf{p}^I) = \{[\exp \operatorname{ad} \mathbf{B}(H_0(t), t, t_0)]f\}(\mathbf{q}^0, \mathbf{p}^0), \qquad \text{(A6)}$$

and, with the correspondence (4.1), yields

$$f(q^I, p^I) = \{[\exp \operatorname{ad} B(H_0(t), t, t_0)]f\}(q^0, p^0). \qquad \text{(A7)}$$

Equations (A5) and (4.13) yield

$$f(\mathbf{q}, \mathbf{p}) = \{[\exp \operatorname{ad} \mathbf{B}(H_1^I(t), t, t_0)]f\}(\mathbf{q}^I, \mathbf{p}^I), \qquad \text{(A8)}$$

whose classical counterpart, obtained with (4.1), is

$$f(q, p) = \{[\exp \operatorname{ad} B(H_1^I(t), t, t_0)]f\}(q^I, p^I). \qquad \text{(A9)}$$

Parenthetically, we remark that since the $\mathbf{q}_i^I$'s and $\mathbf{p}_i^I$'s in (A8) are time dependent, the $\mathbf{q}_i^I$'s at different times do not usually commute, nor do the $\mathbf{p}_i^I$'s. Similarly, in (A9), the Poisson bracket of q_i^I's at different times usually does not vanish, nor does that of the p_i^I's. In contrast, since the $\mathbf{q}^M$ and $\mathbf{p}^M$ in (3.4) are treated as constants in (3.4), the problem of lack of commutativity does not arise in (4.6). Related remarks apply to the latter's classical counterpart (3.8).

Finally, we note that in addition to the Heisenberg, Schrödinger, interaction, and mixed-interaction pictures there are, of course, an infinitude of others, all related by unitary transformations, but the present fourth one bears a particularly symmetrical relationship to the other three.

APPENDIX B: NOTATION

Any notation in a physical article usually involves some compromise between precision, brevity, and clarity. We employ the following notation, one which adapts that in Ref. 21 to the present topic.

Each problem, classical or quantum, in the variation-of-constants method is subdivided into two problems: The first, which is connected with an evolution under the influence of a Hamiltonian $H_0(t)$, and the second, which is connected with an evolution under the influence of a Hamiltonian $H_1^I(t)$. The following remarks are couched in terms of the symbols used for the first problem, but they apply to the second problem after a straightforward relabeling of symbols [q^M's and p^M's replaced by q^0's and p^0's; q's and p's replaced by q^M's and p^M's; $T^*(t)$ changed from meaning exp ad $B(H_0(t), t, t_0)$ to meaning exp ad $B(H_1^I(t), t, t_0)$]. The remarks are also immediately transposed into the quantum-mechanical symbols. In particular, the evolution referred to then is to that of the operators $\mathbf{q}(t)$, $\mathbf{p}(t)$, $\mathbf{q}^M(t)$, $\mathbf{p}^M(t)$, etc.

We begin with a $2N$-dimensional phase space with coordinates $q_i, \cdots q_N p_1 \cdots p_N$. The coordinates could be transformed, if one wished, into some new set of coordinates, $q_1', \cdots p_N'$, and any point or any curve in the space is invariant to such changes. On this phase space are defined functions f. The value of f at some point (q, p) is $f(q, p)$. A dynamical path in the phase space is described by specifying a mapping $t \rightarrow (q(t), p(t))$. If the initial point on such a path $(q(t_0), p(t_0))$ is denoted by (q^M, p^M), then one can introduce an operator $T(t)$ which maps the point (q^M, p^M) into a point (q, p) at a later time t,

$$q_i = T(t) q_i^M, \quad p_i = T(t) p_i^M. \qquad \text{(B1)}$$

One can also describe this evolution by an operator $T^*(t)$ which acts on the space of functions f:

$$f(q, p) = (T^*(t) f)(q^M, p^M), \qquad \text{(B2)}$$

where q and p are $q(t)$ and $p(t)$. An example of (B2) is

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the choice of f to be q_i or p_i. We then have

$$q_i=(T^*(t)q_i)(q^M,p^M),\quad p_i=(T^*(t)p_i)(q^M,p^M), \tag{B3}$$

where the q_i and p_i on the left-hand side describe $q_i(t)$ and $p_i(t)$. The q_i and p_i on the right-hand side describe particular f's.

While $T(t)$ acts directly on points of the phase space, $T^*(t)$ acts on functions f, including "constant functions" q_i and p_i. Following one typical usage in mathematics, the starred notation is reserved for operators acting on functions. (The asterisks could therefore have been added to some other symbols which act on f in this paper, for consistency.)

There is, of course, some possibility of confusion in the above notation, i.e., q_i and p_i have the following two meanings:

(i) They are coordinates of the phase space and, as such, describe any point in that space. Except where they appear as initial points [in which case they denote $q_i(t_0)$ and $p_i(t_0)$], they can be regarded as abbreviations for $q_i(t)$ and $p_i(t)$; for example, in $f(q,p)$ in Eq. (3.4) or in the left-hand sides of Eqs. (B1)–(B3).

(ii) They are examples of "constant functions" f, as in their usage in $T^*(t)q_i$ and $T^*(t)p_i$ in Eq. (B1).

The meaning (ii) should involve no confusion in the main body of text, since f is always used there instead of the symbol q_i or p_i in that context. To apply the equations of the text to obtain $q_i(t)$ and $p_i(t)$, the functions $f=q_i$ and $f=p_i$ are used together with (B3).

The double meaning, (i) and (ii), could be avoided by using additional notation. For example, if a path starting at (q^M,p^M) were denoted by $\alpha_{(q^M,p^M)}(t)$,[21] then $f(q,p)$ could be written as $f(\alpha_{(q^M,p^M)}(t))$, and one would replace (B1) by

$$f(\alpha_{(q^M,p^M)}(t))=(T^*(t)f)(q^M,p^M). \tag{B4}$$

However, even here, the notation in (B3) is so convenient that its equivalent is used in Ref. 21(b).

APPENDIX C: NOTATIONAL COMPARISON WITH REF. 4

In Ref. 4, a common notation was employed. The present paper uses the more modern notation discussed in Appendix B, one which has a conceptual advantage in that it leads to coordinate-free results. An operator $D(t)$ defined in Eq. (B3) of Ref. 4 would, in present notation, when operating on a function f and then evaluated at $\bar{x}$, yield $(D(t)f)(\bar{x})$, defined by

$$(D(t)f)(\bar{x})\equiv\sum\bar{h}_i(\bar{x},t)\partial f(\bar{x})/\partial\bar{x}_i. \tag{C1}$$

Equations (4)–(6), (10), and (24) of Ref. 4 would be written as the following:

$$df(\bar{x})/dt=(D(t)f)(\bar{x}),\qquad t\geq t_0, \tag{C2}$$

$$\bar{x}_i=\bar{x}_i^0,\qquad t=t_0,$$

$$f(\bar{x})=[(\exp(t-t_0)D)f](\bar{x}^0), \tag{C3}$$

$$f(\bar{x})=(\exp\mathcal{O}(t)f)(\bar{x}^0), \tag{C4}$$

$$[(d\mathfrak{D}(t)/dt)f](\bar{x}^0)=(\mathfrak{D}(t)D(t)f)(\bar{x}^0), \tag{C5}$$

$$f(\bar{q},\bar{p})=(\exp\mathcal{O}(t)f)(\bar{q}^0,\bar{p}^0). \tag{C6}$$

* Acknowledgment is made to the donors of the Petroleum Research Fund, administered by the American Chemical Society, for partial support of this research. This research was also supported by a grant from the National Science Foundation at the University of Illinois.

[1] For example, J. M. Jauch, *Foundations of Quantum Mechanics* (Addison–Wesley, Reading, Mass., 1968), pp. 156–157.

[2] For example, E. W. Brown and C. A. Shook, *Planetary Theory* (Cambridge U. P., London, 1933), p. 125; W. M. Smart, *Celestial Mechanics* (Longmans Green, New York, 1953), p. 159.

[3] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Oxford U. P., New York, 1958), 4th ed., p. 174; L. Pauling and E. B. Wilson, Jr., *Introduction to Quantum Mechanics* (McGraw-Hill, New York, 1935), p. 294.

[4] R. A. Marcus, J. Chem. Phys. **52,** 4803 (1970). [In Eq. (4) the $\bar{x}_i=\bar{x}_i$ should read $\bar{x}_i=\bar{x}_i^0$.] Several notational differences occur; e.g., subscripted M quantities here were denoted by barred quantities there. The ad B notation, given later in the present (3.7)–(3.12), replaces $\{B,\quad\}$, etc. A notational difference in writing the equations is described in the present Appendix C.

[5] Reference 3, p. 87. An example of application of the correspondence to the unintegrated equations of motion is given in W. H. Louisell, *Radiation and Noise in Quantum Electrons* (McGraw-Hill, New York, 1964), p. 60.

[6] A. Messiah, *Quantum Mechanics* (North-Holland, Amsterdam, 1961), p. 322.

[7] A. Messiah, Ref. 6, p. 723.

[8] R. G. Newton, *Scattering of Waves and Particles* (McGraw-Hill, New York, 1966), Sec. 6.5, p. 176.

[9] This function arose by converting Eqs. (3.4) and (3.5) to operator equations,[4] and applying a solution to the latter due to W. Magnus, Commun. Pure Appl. Math. **7,** 649 (1954).

[10] J. G. Belinfante, B. Kolman, and H. A. Smith, SIAM Rev. **8,** 1 (1966). In the present instance of Eq. (4) the Poisson bracket is the Lie bracket.

[11] The solution of W. Magnus[9] is applied to (4.11), using the definition of **B** in the present Eq. (4.4).

[12] $(\exp \text{ad } A)\ C=(\exp A)\ C\exp(-A)$; cf. W. H. Louisell, Ref. 5, p. 101; J. Wei and E. Norman, J. Math. Phys. **4,** 575 (1963).

[13] Reference 9, p. 661. Also see, E. Wichmann, J. Math. Phys. **6,** 875 (1961).

[14] W. Magnus, Ref. 9.

[15] N. Jacobson, *Lie Algebras* (Interscience, New York, 1962), p. 7, where the definition is given in terms of multiplication on the right.

[16] Reference 15, pp. 3, 10.

[17] Reference 15, p. 9.

[18] If the equation solved in Ref. 9 is denoted by $dY/dt=A(t)Y$, then differentiation of $YY^{-1}=1$ yields $dY^{-1}/dt=-Y^{-1}A(t)$.

[19] One Lie Algebra is generated by ad $H_1{}^I(t)$ [cf. Eq. (4.3), with $H_1(q,p,t)$ written as $H_1{}^I(q^M,p^M,t)$, and the other is generated by $H_1{}^I(t)$ (Eqs. 4.10 and 4.12)]. "Adjoint representation" is defined in Ref. 10, p. 23.

[20] R. Hermann, *Differential Geometry and the Calculus of Variations* (Academic, New York, 1968), p. 88 for definition of adjoint group.

[21] (a) K. T. Chen, Bull. Am. Math. Soc. **68,** 341 (1962); see also, R. Hermann, Ref. 20, Chap 6; (b) K. T. Chen, Arch. Ratl. Mech. Anal. **13,** 348 (1963).

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